

University of Groningen

Structural classification of the amide I sites of a beta-hairpin with isotope label 2DIR spectroscopy

Roy, Santanu; Jansen, Thomas L. C.; Knoester, Jasper

Published in:
Physical Chemistry Chemical Physics

DOI:
[10.1039/b925645h](https://doi.org/10.1039/b925645h)

IMPORTANT NOTE: You are advised to consult the publisher's version (publisher's PDF) if you wish to cite from it. Please check the document version below.

Document Version
Publisher's PDF, also known as Version of record

Publication date:
2010

[Link to publication in University of Groningen/UMCG research database](#)

Citation for published version (APA):

Roy, S., Jansen, T. L. C., & Knoester, J. (2010). Structural classification of the amide I sites of a beta-hairpin with isotope label 2DIR spectroscopy. *Physical Chemistry Chemical Physics*, 12(32), 9347-9357. <https://doi.org/10.1039/b925645h>

Copyright

Other than for strictly personal use, it is not permitted to download or to forward/distribute the text or part of it without the consent of the author(s) and/or copyright holder(s), unless the work is under an open content license (like Creative Commons).

The publication may also be distributed here under the terms of Article 25fa of the Dutch Copyright Act, indicated by the "Taverne" license. More information can be found on the University of Groningen website: <https://www.rug.nl/library/open-access/self-archiving-pure/taverne-amendment>.

Take-down policy

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

Downloaded from the University of Groningen/UMCG research database (Pure): <http://www.rug.nl/research/portal>. For technical reasons the number of authors shown on this cover page is limited to 10 maximum.

Structural classification of the amide I sites of a β -hairpin with isotope label 2DIR spectroscopy

Santanu Roy, Thomas L. C. Jansen,^{*} and Jasper Knoester[†]

April 15, 2010

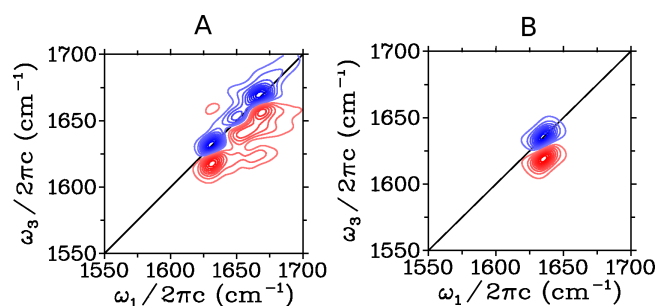


Fig. 1 S: 2DIR spectrum (parallel polarization) of trpzip2 with the T10 site labeled with $^{13}\text{C}^{16}\text{O}$ (A) and 2DIR spectrum of only the T10 site (B) at pH 2.5. A total of 18 equally spaced contours are plotted between $\pm 10\%$ and $\pm 90\%$ of the most intense peak. Blue contours are negative (simulated emission and bleaching) and red contours are positive (excited state absorption). In A, labeled spectrum for T10 is separated from the main spectrum of trpzip2 and is same as the spectrum for only the T10 site. Therefore, calculating the spectrum for only a particular site suffices for studying site-specific vibrational dynamics.

^{*}E-mail: T.L.C.Jansen@rug.nl

[†]Center for Theoretical Physics and Zernike Institute for Advanced Materials, University of Groningen, Nijenborgh 4, 9747 AG Groningen, The Netherlands

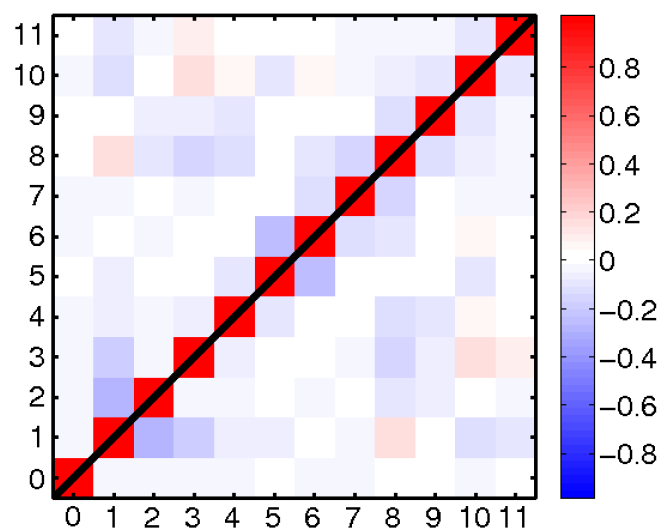


Fig. 2 S: Zero time cross-correlation plot for site frequencies. Red and blue correspond to correlation and anti- correlation, respectively.

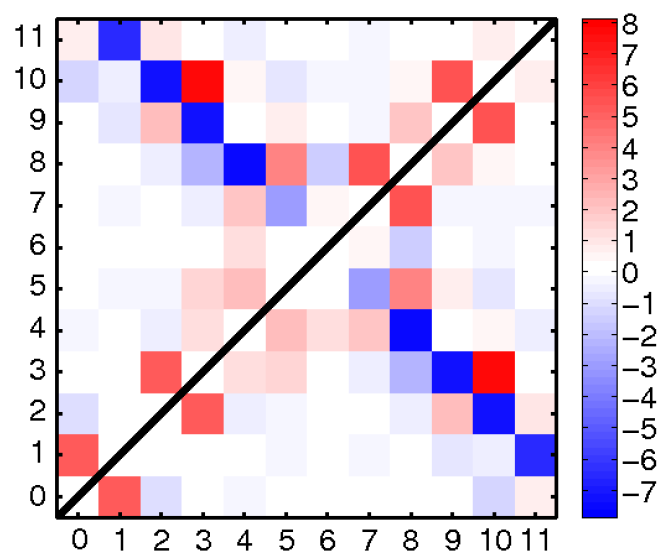


Fig. 3 S: Couplings (J_{ij}) among the sites: blue corresponds to a negative value, while red is positive. The most intense colors have the value of $\pm 7 \text{ cm}^{-1}$.

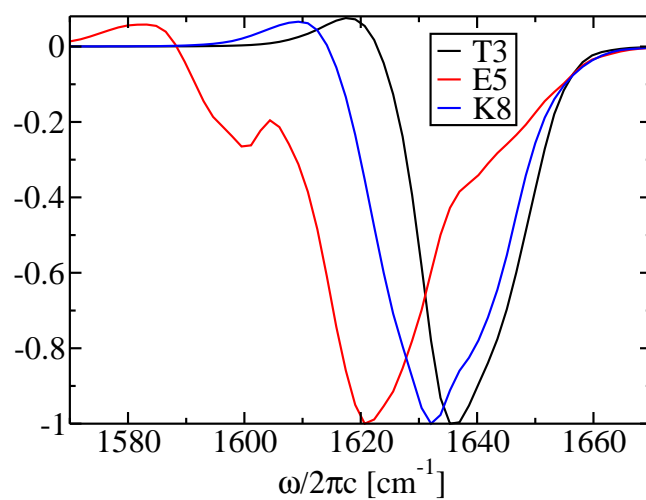


Fig. 4 S: Comparison of the diagonal slices of the 2DIR peaks of T3, E5, and K8.

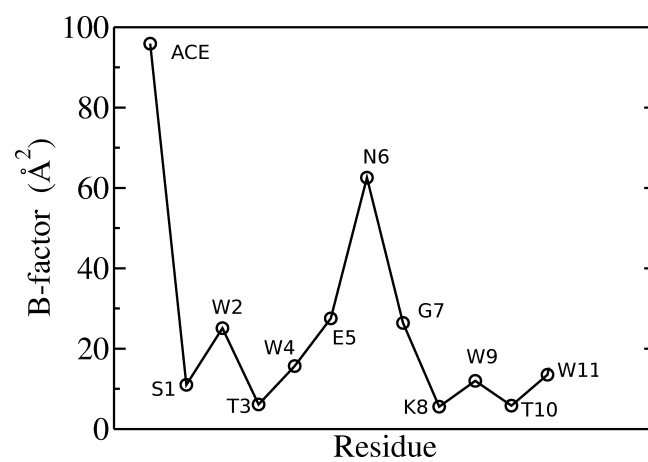


Fig. 5 S: B-factors of the peptide units of trpzip2.